Ignition of Hydrogen-Air Mixtures by Moving Heated Particles

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Caltech
Outline

1. Motivation
2. Previous Work
3. Goal
4. Physical Model, Numerical Approach and Simulation Parameters
5. Results
6. Discussion
7. Closing Remarks
Motivation
Improved understanding of ignition hazards

1. Simulated lightning strike on composite coupon performed at Boeing
2. Mechanical sparks from cutting and reshaping processes
3. Hot particles of decomposed explosive and casing
Outline

1 Motivation

2 Previous Work

3 Goal

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6 Discussion

7 Closing Remarks
Classical Experimental Work
In the 1930’s motivated by coal-mining operations - frictional sparks (moving heated particles)

Figure 5 : effect of particle diameter

Experimental work

More Recent Experimental Work
Ignition of gaseous mixtures by submillimeter size stationary hot particles

Figure 2b: effect of particle material

Figure 4: effect of mixture concentration

Experimental work

Previous & Current Experimental Efforts at Caltech
Ignition of $n$-hexane mixtures

Figure 3.15: transiently heated surfaces

Figure: moving heated spheres

Numerical work

Some Previous & Current Numerical Efforts
1D Simulation assuming spherical symmetry, quiescent atmosphere and no-thermally induced convection

Figure 3b: Effect of mixture concentration\(^6\)

Figure 8: Effect of particle size\(^7\)

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Theoretical Work

Analysis

- C.K. Law\textsuperscript{8} - Stagnation-point ignition of a premixed combustible and ignition of a combustible by hot particles (B.L. equations, one-step irreversible reaction and high activation energy limit)

- Y. B. Zel’dovich\textsuperscript{9} - Ignition of a fuel mixture flowing around an object (B.L. equations, one-step irreversible reaction, Dorodnitsyn transformation, no assumptions made w.r.t. activation energies, complete analytical investigation of the system was impossible)

- More recently Golovin, A.M. and Golovin, A.M & Rudakova, N.B.\textsuperscript{10} with similar simplifying assumptions ...

\textsuperscript{9} The Mathematical Theory of Combustion and Explosions, 1985.
\textsuperscript{10} High Temperature, 1996/1998.
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Goal

Objective

- Explain the dynamics of ignition of combustible gases by inert moving heated spheres when close and far from the ignition limit.
- Study the competition between diffusive and convective losses, and chemical heat release to unravel the complex physics and chemistry at play within the boundary layer during the ignition process.
- Explore the quantitative prediction of ignition thresholds.
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Physical Model - Governing Equations

Reactive Navier-Stokes with temperature dependent properties
($\mu$ : Sutherland Law, $\alpha = k/c_p$ : Eucken Relation, $c_p$ : JANAF)

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\]

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \tau + \rho \mathbf{g}
\]

\[
\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot (\kappa/c_p \nabla h) + q_{chem}, \quad (Le = 1)
\]

\[
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) = \nabla \cdot (\rho D_i \nabla Y_i) + \Omega_i
\]

with $p = \rho \bar{R}T$, $\tau = (p + \frac{2}{3} \mu \nabla \cdot \mathbf{u}) \mathbf{l} + \mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$

\[
h = \sum h_i Y_i, \quad q_{chem} = \sum h_i \Omega_i, \quad \Omega_i = \rho dY_i/dt\]
Challenges

- Wide range of temporal and spatial scales involved
  - Size of experimental apparatus ($O(m)$)
  - Hydrodynamic length scales - Boundary layer thickness ($O(\mu m) - O(mm)$)
  - Chemical induction/ignition times ($O(s)/O(ms)$) and flame thickness ($O(\mu m)$)

- Size of detailed chemical kinetic mechanisms
  - Hydrocarbon fuels conventionally used for transportation comprise thousands of reactions and hundreds of species (e.g. $n$-hexane detailed mechanism: 2581 reactions and 457 species)
Physical Model - Hydrogen Chemistry

Mével’s Mechanism (9 species and 21 reactions)\textsuperscript{11}

Approach

- 2D simulation of reactive viscous flow using the Open source Field Operation And Manipulation (OpenFOAM) toolbox
- Spatial discretization done with Finite Volumes (FV)
- Pressure-velocity coupling achieved using PIMPLE (PISO + SIMPLE)
- Implementation of time dependent boundary conditions to reproduce actual experimental conditions
- High Performance Computing - resources provided by the Extreme Science and Engineering Discovery Environment (XSEDE) supported by the National Science Foundation (NSF)

Experimental setup, initial & boundary conditions

- **Outflow**
  - $p_o = 100$ kPa
  - $T_o = 300$ K
  - $u_o = (0, 0, 0)$ m/s
  - $Y_{N2} = 1$

- **Inflow**
  - $u(t) = (0, gt, 0)$ m/s

- **At wall**
  - $T = T_{sphere}$
  - $u = (0, 0, 0)$ m/s

- **Reactive Mixture**
  - $Y_{N2} = 0.0283$
  - $Y_{O2} = 0.2264$
  - $Y_{N2} = 0.7453$

- **Supports**
- **Optical Shutter**
- **Window**
- **Pyrometer**
- **N2 Line**
- **Pneumatic Actuator**
- **Sphere**
Nature of flow before contact with reactive mixture

Recirculation zone (wake)

Separation region

Boundary layer growth

Front stagnation point

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Comparison with non-reactive experiments
Flow structure - boundary layer development

Temperature and velocity fields, temperature isocontours and streamlines before contact with reactive mixture
When does ignition take place?

Temperature maximum in computational domain

\[ \tau_{\text{ign}} = T_{\text{sphere}} + 150 \text{K} \]
When does ignition take place?

Temperature maximum in computational domain

\[ \tau_{\text{ign}} = T_{\text{sphere}} + 150K \]
When does ignition take place?

Temperature maximum in computational domain:

\[ \tau_{ign} = T_{sphere} + 150K \]
Where does ignition take place? (1/8)

$T_{\text{sphere}} = 1200 \text{ K} - \text{Ignition Evolution}$

$t = 0.25237 \text{ s}$
$t = 0.25250 \text{ s}$
$t = 0.25275 \text{ s}$
$t = 0.2530 \text{ s}$

Shortly before ignition
Ignition
Flame kernel formation
Flame propagation
Where does ignition take place? (2/8)

$T_{\text{sphere}} = 1200 \text{ K}$

Closeup to ignition location - $\theta = 0^\circ$
Where does ignition take place? (3/8)

\[ T_{\text{sphere}} = 1000 \text{ K} - \text{Ignition Evolution} \]

- \( t = 0.254354 \text{ s} \) Shortly before ignition
- \( t = 0.254386 \text{ s} \) Ignition
- \( t = 0.254466 \text{ s} \) Flame kernel formation
- \( t = 0.25475 \text{ s} \) Flame propagation

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Where does ignition take place?

$T_{\text{sphere}} = 1000 \text{ K}$

Closeup to ignition location - $\theta = 90^\circ$
Where does ignition take place? (5/8)

$T_{\text{sphere}} = 960$ K - Ignition Evolution

- $t = 0.26625 \text{ s}$: Shortly before ignition
- $t = 0.266306 \text{ s}$: Ignition
- $t = 0.266362 \text{ s}$: Flame kernel formation
- $t = 0.2665 \text{ s}$: Flame propagation
Where does ignition take place? (6/8)

\[ T_{\text{sphere}} = 960 \text{ K} \]

Closeup to ignition location - \( \theta = 115^\circ \) (threshold)
Where does ignition take place?

$T_{\text{sphere}} = 950 \text{ K} - \text{No Ignition}$

$t = 0.255 \text{ s}$

$t = 0.260 \text{ s}$

$t = 0.265 \text{ s}$

$t = 0.270 \text{ s}$
Where does ignition take place?

$$T_{\text{sphere}} = 950 \, \text{K}$$

No Ignition
Results Summary

Ignition times and locations from 2D simulations
Discussion

Ignition times analysis

Comparison of 2D and constant pressure ignition times
Ignition times analysis

Comparison of 2D and constant pressure ignition times

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Ignition times analysis

Comparison of 2D and constant pressure ignition times

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Ignition times analysis

Comparison of 2D and constant pressure ignition times

\[ \tau_{\text{ign}} \text{ 2D} \]
\[ \tau_{\text{ign}} \text{ 0D} \]
Ignition times analysis

Comparison of 2D and constant pressure ignition times
Discussion

Ignition times analysis

Comparison of 2D and constant pressure ignition times

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Recall the energy equation

\[
\frac{\partial (\rho h)}{\partial t} = -\nabla \cdot (\rho \mathbf{u} h) + \nabla \cdot \left( \frac{\kappa}{c_p} \nabla h \right) - q_{chem}
\]

- **Sum (---)**
- **hConvection (→)**
- **hDiffusion (→)**
- **hSource (→)**
Energy equation analysis (2/5)

\[ T_{\text{sphere}} = 1200 \text{ K} \]

Closeup to ignition location - \( \theta = 0^\circ \)
Discussion

Energy equation analysis (2/5)

$T_{\text{sphere}} = 1200 \text{ K}$

Closeup to ignition location - $\theta = 0^\circ$
 Contributions of each term in energy equation and temperature along radial distance from sphere’s surface
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Energy equation analysis (3/5)

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Energy equation analysis (4/5)

\[ T_{\text{sphere}} = 960 \, \text{K} \]

Closeup to ignition location - \( \theta = 115^\circ \) (threshold)
Energy equation analysis (4/5)

\[ T_{\text{sphere}} = 960 \text{ K} \]

Closeup to ignition location - \( \theta = 115^\circ \) (threshold)
Contributions of each term in energy equation and temperature along radial distance from sphere's surface
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- Contributions of each term in energy equation and temperature along radial distance from sphere’s surface.

4 mm Sphere @ 960 K - $\theta = 115$

Temperature (K)

$\delta = 2 \text{ mm}$

Ign. Loc : $0.04\delta, r = 0.08 \text{ mm}$

Contributions of each term in energy equation and temperature along radial distance from sphere’s surface.
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Contributions of each term in energy equation and temperature along radial distance from sphere’s surface
Temporal evolution near ignition location

$T_{\text{sphere}} = 1200 \text{ K}$

Closeup to ignition location - $\theta = 0^\circ$
Temporal evolution near ignition location (2/2)

Temporal Evolution of each term in energy equation, temperature and species mass fractions at the ignition location
Temporal evolution near ignition location (2/2)

Temporal Evolution of each term in energy equation, temperature and species mass fractions at the ignition location
Temporal evolution near ignition location (3/4)

$T_{\text{sphere}} = 960 \text{ K}$

Closeup to ignition location - $\theta = 115^\circ$ (threshold)
Temporal Evolution of each term in energy equation, temperature and species mass fractions at the ignition location
Temporal evolution near ignition location (4/4)

Temporal Evolution of each term in energy equation, temperature and species mass fractions at the ignition location.
**Chemical Pathways**

\[
\begin{align*}
T_{sphere} &= 1200K \\
T_{sphere} &= 960K
\end{align*}
\]

Box: Species Reservoirs
- Solid line: Reservoir Inputs
- Dashed line: Reservoir Outputs

- Pink: Chain-branching
- Gray: Mixed pathways
- Green: Non-chainbranching

**At high T:**
- OH radicals mostly produced by chain-branching processes (77%)
- R1: \( \text{O}_2 + \text{H} = \text{OH} + \text{O} \)
- R2: \( \text{H}_2 + \text{O} = \text{H} + \text{OH} \)
- Non-chain branching through Path 1 (23%)

**At low T:**
- Chain-branching processes significantly less (42%)
- Non-chain branching processes
  - Path 1 (38%)
    - R5: \( \text{H} + \text{O}_2(\pm \text{M}) = \text{HO}_2(\pm \text{M}) \)
    - R3: \( \text{HO}_2 + \text{H} = \text{OH} + \text{OH} \)
  - Path 2 (16%)
    - R6: \( \text{H} + \text{O}(\pm \text{M}) = \text{OH}(\pm \text{M}) \)

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**Chemical Pathways**

At high T:
OH radicals mostly produced by chain-branching processes (77%)
- \( R_1 : O_2 + H = OH + O \)
- \( R_2 : H_2 + O = H + OH \)
Non-chain branching through Path 1 (23%)

At low T:
Chain-branching processes significantly less (42%)
Non-chain branching processes

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**Chemical Pathways**

**At high T:**
OH radicals mostly produced by chain-branching processes (77%)
- $R_1: O_2 + H = OH + O$
- $R_2: H_2 + O = H + OH$
Non-chain branching through Path 1 (23%)

**At low T:**
Chain-branching processes significantly less (42%)
Non-chain branching processes
- **Path 1 (38%)**:
  - $R_5: H + O_2(+M) = HO_2(+M)$
  - $R_3: HO_2 + H = OH + OH$
- **Path 2 (16%)**:
  - $R_6: H + O(+M) = OH(+M)$

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**Tsphere = 1200K**
**Tsphere = 960K**

**Box:** Species Reservoirs
- **Chain-branchning**: ---
- **Mixed pathways**: ----
- **Non-chainbranching**: ---

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Quantitative prediction of ignition thresholds for hot surfaces require a detailed model that includes correct initial and boundary conditions to capture important features such as boundary layer separation, and energy transport processes.

Ignition occurs within the thermal boundary layer at a location that depends strongly on temperature.

Large differences observed between 2D and 0D ignition times suggests that simplified models based on comparison of residence times with ignition delay times are inappropriate.

As the temperature decreases to the ignition threshold, non-chain branching chemical pathways are favored over chain branching processes.
Two distinct behaviors observed:

- Far from the ignition threshold
  - Reaction starts shortly after contact with reactive mixture
  - Ignition occurs between the front stagnation point and separation region depending upon the sphere’s surface temperature
  - Ignition time is very short and takes place in a more diluted mixture compared cases close to the ignition threshold

- Closer to the threshold
  - Rate of heat deposition into the gas not high enough to trigger fuel conversion during transit from the front stagnation point to the separation region
  - Boundary layer separation results in a zone of slower moving gas, where reactive mixture is "confined", conduction of heat takes place readily and convective losses are minimal
Not only does flow separation play an important role in hot particle ignition, but also when considering different geometries.